Kinetic and macroscopic diffusion models for gas mixtures in the context of respiration

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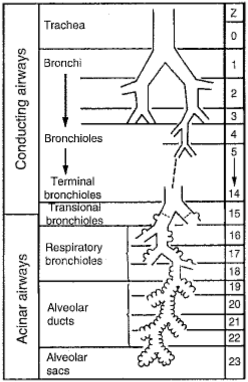
Context of respiration

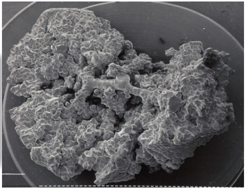
- Modelling air as a mixture of several gases : N_2, O_2, (H_2O)
- In the context of respiration (gaseous exchanges) : CO_2
- For some pathologies $N_2 \longrightarrow$ He
- Expected improvements : respiration & oxygen transfer



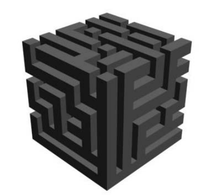
- Decomposition of the respiratory tree in 2 parts
- Bronchi and bronchioles (1st - 16th gen.) : convective regime
- Acini (17th - 23rd gen.) : predominant diffusion and gaseous exchanges

Diffusion for gaseous mixtures

$\rightsquigarrow$ (Cross-)diffusion models

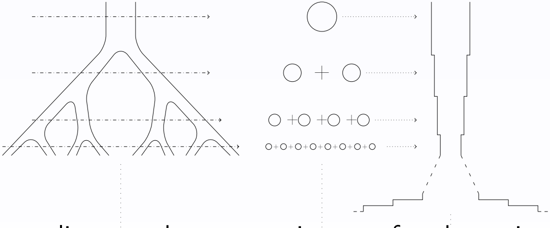


Modelling the respiratory system including lower airways



- Stokes equation with Kitaoka's geometry for acini: MAUROY, FILOCHE, SAPOVAL...
- Alternative: reduced model
  1D domain, longitudinal velocity u

- 0D mechanical model gives the flow
- Discontinuous equivalent section S set with morphometric data



- Mass conservation equation coupling u and concentrations c_i of each species
- Incompressibility
- Convection-diffusion equations: $\partial_t(Sc_i) + \partial_x(Sc_i u) + \partial_x(SN_i) = 0$
- Diffusive fluxes N_i (nonlinearly) linked to the concentration gradients
- Gaseous exchanges taken into account from the 17th generation

Aim of the study

Justification of macroscopic diffusion models for mixtures

- Choice of the (cross-)diffusion model, Justification of the validity regime
- Computations of the physical macroscopic diffusion coefficients

Use the mesoscopic (kinetic) description

- Boltzmann equation for mixtures
- Hydrodynamic limit
  - Formal computations
  - Rigorous convergence
  - Asymptotic-preserving schemes

Two different scales for the description of each species i

- mesoscopic scale (kinetic model): distribution function $f_i(t,x,v)$
- macroscopic scale: physical observables
  - concentration $c_i(t,x)$
  - velocity $u_i(t,x)$

$\rightsquigarrow$ flux of species i : $N_i(t,x) = c_i(t,x)u_i(t,x)$

Properties of the collision operator & Diffusive scaling

Same kinetic setting and notations as in Milana Pavić-Čolić's talk

- Equilibrium: Maxwellian with same bulk velocity and temperature

$$c_i(t,x)\left(\frac{m_i}{2\pi k_B T}\right)^{d/2}\exp\left(-\frac{m_i|v-u(t,x)|^2}{2k_B T}\right)$$

- Conservation properties of the collision operator for $1 \le i,j \le I$

$$\int_{\mathbb{R}^d} Q_{ij}(f_i,f_j)(v)\,\mathrm{d}v = 0 \quad \text{and} \quad \int_{\mathbb{R}^d} Q_{ii}(f_i,f_i)(v)\,v\,\mathrm{d}v = 0.$$

Diffusive scaling

Small mean free path and Mach number: Kn $\sim$ Ma $\sim \varepsilon$

$$\varepsilon\partial_t f_i^\varepsilon + v\cdot\nabla_x f_i^\varepsilon = \frac{1}{\varepsilon}\sum_{j=1}^{I} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon), \qquad 1 \le i \le I$$

Moment method

Moments of the distribution functions

- Concentration of species i

$$c_i^\varepsilon(t,x) = \int_{\mathbb{R}^d} f_i^\varepsilon(t,x,v)\,\mathrm{d}v$$

- Flux of species i

$$N_i^\varepsilon(t,x) = c_i^\varepsilon(t,x)\, u_i^\varepsilon(t,x) = \frac{1}{\varepsilon}\int_{\mathbb{R}^d} v\, f_i^\varepsilon(t,x,v)\,\mathrm{d}v$$

Ansatz

The distribution function of each species i is at a local Maxwellian state with a small different velocity of order ε for any $(t,x) \in \mathbb{R}_+ \times \Omega$

$$f_i^\varepsilon(t,x,v) = c_i^\varepsilon(t,x)\left(\frac{m_i}{2\pi k_B T}\right)^{d/2} \exp\left(-\frac{m_i|v-\varepsilon u_i^\varepsilon(t,x)|^2}{2k_B T}\right)$$

Macroscopic diffusion equations

$$\boxed{\varepsilon \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_j Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)}$$

- Mass conservation: moment of order 0

$$\varepsilon \frac{\partial}{\partial t} \left(\int_{\mathbb{R}^3} f_i^\varepsilon(v) \, \mathrm{d}v \right) + \nabla_x \cdot \left(\int_{\mathbb{R}^3} v \, f_i^\varepsilon(v) \, \mathrm{d}v \right) = 0,$$

where the collision term vanishes (conservation property).

- Momentum equation: moment of order 1

$$\varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^3} v \, f_i^\varepsilon(v) \, \mathrm{d}v + \int_{\mathbb{R}^3} v \, \left(v \cdot \nabla_x f_i^\varepsilon(v) \right) \, \mathrm{d}v = \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^3} v \, Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)(v) \, \mathrm{d}v$$

where the mono-species collision term vanishes (conservation property).

Computation of the divergence term

$$\varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^3} v \, f_i^\varepsilon(v) \, dv + \boxed{\int_{\mathbb{R}^3} v \, \left(v \cdot \nabla_x f_i^\varepsilon(v)\right) \, dv} = \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^3} v \, Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)(v) \, dv$$

- Use of the Ansatz, translation in v + parity argument

$$\nabla_x \cdot \left(\int v \otimes v \, f_i^\varepsilon(v) \, \mathrm{d}v \right) \propto \nabla_x \cdot \left(c_i^\varepsilon \int \left(v \otimes v + \varepsilon^2 u_i^\varepsilon \otimes u_i^\varepsilon \right) e^{-m_i |v|^2 / 2 k_B T} \mathrm{d}v \right)$$

- In terms of macroscopic quantities

$$\nabla_x \cdot \left(\int v \otimes v \, f_i^\varepsilon(v) \, \mathrm{d}v \right) = \frac{k_B T}{m_i} \nabla_x c_i^\varepsilon + \varepsilon^2 \nabla_x \cdot \left(c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon \right)$$

Computation of the collision term

- For Maxwell molecules $\mathcal{B}_{ij} = b_{ij}(\cos\theta)$

  weak form, collision rules, symmetry and parity arguments

$$\int v\, Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)(v)\,\mathrm{d}v = \frac{m_j}{m_i+m_j}\int b_{ij}(\cos\theta)\, f_i^\varepsilon f_{j*}^\varepsilon\,(v_* - v + |v - v_*|\sigma)\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v$$

  In terms of macroscopic quantities

$$\frac{1}{\varepsilon}\sum_{j\neq i}\int v\, Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)(v)\,\mathrm{d}v = \sum_{j\neq i}\underbrace{\frac{2\pi m_i m_j \|b_{ij}\|_{L^1}}{(m_i+m_j)k_B T}}_{D_{ij}^{-1}}\frac{k_B T}{m_i}\Big(c_i^\varepsilon c_j^\varepsilon u_j{}^\varepsilon - c_j^\varepsilon c_i^\varepsilon u_i{}^\varepsilon\Big)$$

- For general cross sections: algebraic arguments [Boudin, G., Pavan, '17]

Formal asymptotics and limit equation

Formal limit

$$c_i(t,x) = \lim_{\varepsilon\to 0} c_i^\varepsilon(t,x), \qquad N_i(t,x) = \lim_{\varepsilon\to 0} c_i^\varepsilon(t,x) u_i^\varepsilon(t,x)$$

- Mass conservation

$$\partial_t c_i + \nabla_x \cdot N_i = 0$$

- Momentum equation (order ε^0)

$$\varepsilon^2 \frac{m_i}{k_B T}\Big(\partial_t (c_i^\varepsilon u_i^\varepsilon) + \nabla_x \cdot (c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon)\Big) + \nabla_x c_i^\varepsilon = \sum_{j\neq i} \frac{c_i^\varepsilon c_j^\varepsilon u_j^\varepsilon - c_j^\varepsilon c_i^\varepsilon u_i^\varepsilon}{D_{ij}} + o(1)$$

Maxwell-Stefan equations

$$-\nabla_x c_i = \sum_{j\neq i} \frac{c_j N_i - c_i N_j}{D_{ij}}$$

Rigorous convergence [A. Bondesan's PhD thesis]

Perturbative setting

- Expansion around a Maxwellian M_i: $\boxed{f_i^\varepsilon = M_i + \varepsilon g_i^\varepsilon}$
- Linearized (around M_i) Boltzmann operator $\mathcal{L}_i$
- In the (scaled) Boltzmann equation, it gives

$$\varepsilon \partial_t g_i^\varepsilon + v \cdot \nabla_x g_i^\varepsilon = \frac{1}{\varepsilon} \mathcal{L}_i(g^\varepsilon) + \sum_j Q_{ij}(g_i^\varepsilon, g_j^\varepsilon) + S_i^\varepsilon$$

with $S_i^\varepsilon = \partial_t M_i + \frac{1}{\varepsilon} v \cdot \nabla_x M_i + \frac{1}{\varepsilon^2} \sum_j Q_{ij}(M_i, M_j)$

Monospecies case with $M_i = \mu_i$ global Maxwellian (equilibrium)

$$\mu_i = \bar{c}_i (m_i / 2\pi k_B T)^{d/2} e^{-m_i |v|^2 / 2 k_B T}$$

$\rightsquigarrow$ $Q_{ij}(M_i, M_j) = 0$

$\rightsquigarrow$ $S_i^\varepsilon = 0$

Importance of the spectral gap

Main ingredient : Spectral gap on the linearized Boltzmann operator $\mathcal{L}_i$
$\rightsquigarrow$ Control of the nonlinear term

- Multiply the Boltzmann equation by $g_i \mu^{-1}$, leading order

$$\partial_t \|g_i\|^2_{L^2_v(\mu^{-1})} + \nabla_x \cdot \int v g_i^2 \mu^{-1} dv = \langle g_i, \mathcal{L}_i(g) \rangle_{L^2_v(\mu^{-1})}{}^{(\dagger)}$$

- Spectral gap $\rightsquigarrow$ Coercivity estimate

$$\langle g_i, \mathcal{L}_i g \rangle_{L^2_v(\mu^{-1})} \leq -\lambda_{\mathcal{L}} \|g_i - \pi_{\mathcal{L}} g_i\|_{L^2_v(\mu^{-1})}{}^{(\dagger\dagger)}$$

$\rightsquigarrow$ Global existence, uniqueness, and convergence to equilibrium

Explicit exponential convergence via hypocoercivity methods

$\rightsquigarrow$ Convergence in the hydrodynamic limit

(†) Weighted space $L^2(w)$ defined by the scalar product $\langle f, g \rangle_{L^2_v(w)} = \int f\, g\, w \, \mathrm{d}v$

(††) Projection $\pi_{\mathcal{L}} g_i$ of g_i on $\mathrm{Ker}\, \mathcal{L}$

Multispecies context

Choice of the Maxwellian

Local Maxwellian (not an equilibrium) with different velocities (cf. Ansatz)

- Problem to control the stiff source term
- Linearized Boltzmann operator $\mathcal{L}^\varepsilon$ not self-adjoint
- Problem to describe $\operatorname{Ker} \mathcal{L}^\varepsilon$

- Write $M_i^\varepsilon = \mu_i + (M_i^\varepsilon - \mu_i) = \mu_i + \mathcal{O}(\varepsilon)$
  - Suitable choice of the macroscopic quantities $(c_i,\, u_i)$
  - ✓ Check that $S^\varepsilon = \mathcal{O}(1)$
- Spectral gap property for the operator $\mathcal{L}^\varepsilon$ up to a correction of order ε

$$\langle f, \mathcal{L}^\varepsilon f \rangle_{L^2_v(\mu^{-1})} \leq -(\lambda_{\mathcal{L}} + C\varepsilon) \| f - \pi_{\mathcal{L}} f \|_{L^2_v(\langle v \rangle^\gamma \mu^{-1})} + C\varepsilon \| \pi_{\mathcal{L}} f \|_{L^2_v(\langle v \rangle^\gamma \mu^{-1})}$$

- Write $\mathcal{L}_i^\varepsilon = \mathcal{L}_i + \mathcal{L}_i^\varepsilon - \mathcal{L}_i$
- Pointwise estimate

$$|M_i^\varepsilon - \mu_i| \leq C\varepsilon c_i^{1-\delta} |u_i| \mu_i^\delta$$

- $\mathcal{L}_i^\varepsilon - \mathcal{L}_i$ written as a multiplicative operator + operator in kernel form

Thank you for your attention!

- Hydrodynamic limit from Boltzmann equation for mixtures
- Context of respiration

- ? Complex geometry
- ? Polyatomic gases
- ? Non-isothermal setting